Introduction to Chemical Engineering

Chapter 05

Material Balances

(How Much Base Do We Need?)
5.1 Conservation of total mass

- One important principle in dealing with material balances is that total mass is conserved.
- All mass entering a system will either leave that same system or will accumulate in the system.

\[ \text{Rate that mass enters the system} = \text{Rate that mass leaves the system} + \text{Rate that mass accumulates in the system} \]  

(5.1)  

*Unlike total mass, total moles are not always conserved.*

- At steady-state process,

\[ \text{Rate that mass enters the system} = \text{Rate that mass leaves the system} + \text{Rate that mass accumulates in the system} \]  

(5.2)
5.1 Conservation of total mass

A schematic diagram of a general system with input and output streams

\[ \dot{m}_1 + \dot{m}_2 + \dot{m}_3 = \dot{m}_4 + \dot{m}_5 + \dot{m}_6 \]

Steady-State Total Mass Balance

\[ \sum_{\text{input streams}} \dot{m}_{\text{in}} = \sum_{\text{output streams}} \dot{m}_{\text{out}} \quad (5.3) \]

\[ \dot{m} = \rho \dot{V} \quad (5.4a) \]

\[ \sum_{\text{input streams}} (\rho \dot{V})_{\text{in}} = \sum_{\text{output streams}} (\rho \dot{V})_{\text{out}} \]

\[ \sum_{\text{input streams}} \dot{m}_{\text{in}} = \sum_{\text{output streams}} (\rho \dot{V})_{\text{out}} \]

\[ \sum_{\text{input streams}} (\rho \dot{V})_{\text{in}} = \sum_{\text{output streams}} \dot{m}_{\text{out}} \]
5.1 Conservation of total mass

**Example 5.2**

Three different streams deliver contaminated oil to a waste oil tank, and the mass or volumetric flow rates of those streams are given below:

<table>
<thead>
<tr>
<th>Input stream</th>
<th>Volumetric flow rate (gal/hr)</th>
<th>Density (lb_m/ft^3)</th>
<th>Mass flow rate (lb_m/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>27.4</td>
<td>53.7</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>243.9</td>
</tr>
<tr>
<td>3</td>
<td>19.4</td>
<td>46.0</td>
<td></td>
</tr>
</tbody>
</table>

If the oil leaving the tank has a density of 50.8 lb_m/ft^3, at what volumetric flow rate must the oil be withdrawn to maintain a constant scale reading?
5.1 Conservation of total mass

Steps for analyzing material balance problems

1. **Draw a diagram** if one is not already available.

2. **Write all known quantities** (flow rates, densities, etc.) in the appropriate locations on the diagram. If symbols are used to designate known quantities, include those symbols on the diagram.

3. **Identify and assign symbols to all unknown quantities** and write them in the appropriate locations on the diagram.

4. **Select a basis if needed**: if no flow rates are known, assume a convenient value for one of the flow rates as a basis of calculation (e.g., 100 lbmol/s, 100 kg/hr, etc.).

5. **Determine the appropriate set of equations** needed to solve for the unknown quantities. In order for the problem to be solved, the number of equations must equal the number of unknowns. The steps below can be used to obtain the desired set of equations.
   a. Construct the material balance equation(s):
      1. Start with the general equation
      2. Discard terms that equal zero in your specific problem
      3. Replace remaining terms with more convenient forms
   b. Construct equations to express other known relationships between variables

6. **Solve algebraically and then numerically**: solve algebraically for the desired parameters and then determine their values.
5.1 Conservation of total mass

**Example 5.3**

Your company uses a process to concentrate orange juice by freeze-drying. The input to the process is orange juice that has a density of 1.01 g/cm³. Two streams are output from the process. The first output stream is the orange juice concentrate. The second is an ice slurry that has a density of 0.93 g/cm³. The orange juice is concentrated such that the volume of the concentrate is \( \frac{1}{4} \) that of the incoming juice. Also, from experience it is known that we want to remove ice slurry at the following volumetric rate (where \( J = \) juice and \( I = \) ice):

\[
\dot{V}_I = 0.7 \frac{\rho_J \dot{V}_J}{\rho_I}
\]

What is the density of the concentrate?
5.2 Material balances for multiple species

Mass balance for species A

At steady-state process,

Steady-State Mass Balance for Species A

\[ \sum_{\text{input streams}} m_{A,in} + R_{\text{formation},A} = \sum_{\text{output streams}} m_{A,out} + R_{\text{consumption},A} \]

(5.7)

\[ R_{\text{formation},A} = \text{rate that species A is formed, in units of mass/time} \]

\[ R_{\text{consumption},A} = \text{rate that species A is consumed, in units of mass/time} \]
5.2 Material balances for multiple species

Example 5.4

Natural gas, which is essentially pure methane, undergoes steady-state combustion by injecting it into a small burner into which air is also injected. The methane flow rates in the steady input and output streams are

- Natural gas input stream: Methane mass flow rate = 4.61 g/s
- Air input stream: Contains no methane
- Output (flue gas) stream: Flow rate of unburned methane = 0.09 g/s

At what rate is the methane being burned (consumed)?
5.2 Material balances for multiple species

Other expressions of mass and molar flow rates

\[
\dot{m}_A = x_A \dot{m} = MW_A \dot{n}_A = MW_A y_A \dot{n} = MW_A c_A \dot{V}
\]

(5.8a)

\[
\dot{n}_A = \frac{\dot{m}_A}{MW_A} = \frac{x_A \dot{m}}{MW_A} = y_A \dot{n} = c_A \dot{V}
\]

(5.8b)

Many forms of the material balance for species A

\[
\sum_{\text{input streams}} \dot{m}_{A,\text{in}} + R_{\text{formation,} A} = \sum_{\text{output streams}} \dot{m}_{A,\text{out}} + R_{\text{consumption,} A}
\]

\[
\sum_{\text{input streams}} MW_A \dot{n}_{\text{in}} + R_{\text{formation,} A} = \sum_{\text{output streams}} MW_A (c_A \dot{V})_{\text{out}} + R_{\text{consumption,} A}
\]

\[
\sum_{\text{input streams}} MW_A (y_A \dot{n})_{\text{in}} + R_{\text{formation,} A} = \sum_{\text{output streams}} \dot{m}_{A,\text{out}} + R_{\text{consumption,} A}
\]

\[
\sum_{\text{input streams}} MW_A (c_A \dot{V})_{\text{in}} + R_{\text{formation,} A} = \sum_{\text{output streams}} x_A \dot{m}_{\text{out}} + R_{\text{consumption,} A}
\]

\[
\cdots\cdots
\]
5.2.1 Material balances with formation or consumption where chemical reaction stoichiometry is not given

Example 5.5

Penicillin is produced in reactors containing the bacteria of the species Penicillium chrysogenum. One such method involves continuous (steady-state) production in a continuously stirred tank reactor, where optimum penicillin production has been reported when both of the following are true:

1. the penicillin concentration inside the reactor is 0.002 $\text{g mol/L}$
2. the inlet volumetric flow rate is 0.25 $L/hr$ for a 10 $L$ reactor

A nutrient stream (containing no penicillin) is fed to a 10 $L$ reactor containing the Penicillium chrysogenum bacteria. A product stream containing penicillin leaves the reactor (the bacteria stay in the reactor, and the penicillin concentration in the product stream is the same as inside the reactor). The densities of the nutrient and product streams can be assumed to be equal.

What is the production rate of penicillin under these conditions?

Note: The molecular weight of this penicillin can be taken as 334.4.
5.2 Material balances for multiple species

5.2.2 Material balances with no formation/consumption

Example 5.6
Benzene and toluene (two similar compounds) are partially separated using a distillation column. The feed (input) stream of 100 kg/hr contains benzene at a mass fraction of 0.40, with the balance being toluene. In the overhead output stream, the benzene flow rate is 36 kg/hr, and in the bottoms output stream, the toluene flow rate is 54 kg/hr. What are the toluene flow rate in the overhead output stream, and the benzene flow rate in the bottoms output stream?
5.2 Material balances for multiple species

5.2.3 Material balances with formation/consumption where chemical reaction stoichiometry is given

- Symbols of formation/consumption rate

\[ r_{\text{formation}, A} = \text{rate that species } A \text{ is formed, in units of moles/time}, \quad R_{\text{formation}, A} = MW_A r_{\text{formation}, A} \]  
\[ r_{\text{consumption}, A} = \text{rate that species } A \text{ is consumed, in units of moles/time}, \quad R_{\text{consumption}, A} = MW_A r_{\text{consumption}, A} \]  

- Steady-State Mole Balance for Species A

\[ \sum_{\text{input streams}} \dot{n}_{A,\text{in}} + r_{\text{formation}, A} = \sum_{\text{output streams}} \dot{n}_{A,\text{out}} + r_{\text{consumption}, A} \]  

Other forms…

\[ \sum_{\text{input streams}} (y_A \dot{n})_{\text{in}} + r_{\text{formation}, A} = \sum_{\text{output streams}} \dot{n}_{A,\text{out}} + r_{\text{consumption}, A} \]

\[ \sum_{\text{input streams}} (c_A \dot{V})_{\text{in}} + r_{\text{formation}, A} = \sum_{\text{output streams}} (y_A \dot{n})_{\text{out}} + r_{\text{consumption}, A} \]
5.2 Material balances for multiple species

5.2.3 Material balances with formation/consumption where chemical reaction stoichiometry is given

- Chemical reaction with stoichiometric coefficients

\[ \nu_A A + \nu_B B \rightarrow \nu_C C + \nu_D D \]

\[ \frac{r_{\text{consumption},B}}{r_{\text{consumption},A}} = \frac{\nu_B}{\nu_A} \]

\[ \frac{r_{\text{formation},C}}{r_{\text{consumption},A}} = \frac{\nu_C}{\nu_A} \]

\[ \frac{r_{\text{formation},D}}{r_{\text{consumption},A}} = \frac{\nu_D}{\nu_A} \]

- Consumption rate of A with the fractional conversion of A

\[ r_{\text{consumption},A} = X_A \sum_{\text{All Input Streams}} \dot{n}_{A,\text{in}} \]

For example, an 85% conversion of A means that 85% of the A that enters the reactor is consumed in the reaction.
5.2 Material balances for multiple species

5.2.3 Material balances with formation/consumption where chemical reaction stoichiometry is given

Example 5.7

Ethylene is used to make many important products, including the common polymer polyethylene (used to make plastic bags and many other products). As a design engineer, you are designing a process to convert some excess butene \((C_4H_8)\) to ethylene \((C_2H_4)\) using the reaction

\[
C_4H_8 \rightarrow 2C_2H_4
\]

Your process will include reaction and separation, and two streams will exit the process: an ethylene-rich stream and a butene-rich stream. The following are requirements for the process:

Feed (input) stream:
- Flow rate: 865 \text{ lb}_m/\text{hr}
- Composition: Pure butene

Ethylene-rich output stream:
- Flow rate: 25.5 \text{ lbmol}/\text{hr}
- Composition: 92 mole\% ethylene (the rest is butene)

Butene-rich output stream:
- Flow rate: 240 \text{ ft}^3/\text{hr}
- Composition: ethylene and butene

Of the incoming butene, 84\% is converted to ethylene. What will be the concentrations of ethylene and butene (in units of \text{ lbmol/ft}^3) in the butene-rich outlet stream?
5.3 Material balances: summary

**Decision-tree diagram**

Material Balance

- Is species information is required, or will a total balance suffice?
  - Total Balance
    - Is Adequate
    - Species Balance(s)
      - Needed
        - No Formation/Consumption
        - Formation/Consumption
          - If there are formation/consumption terms, is the reaction stoichiometry known or unknown?
            - Known Stoichiometry
            - Unknown Stoichiometry
5.3 Material balances: summary

5.3.1 The acid-neutralization problem

\[ \text{HCl} + \text{NaOH} \rightarrow \text{H}_2\text{O} + \text{NaCl} \]

**Steady-State Mole Balance for HCl**

\[
\sum_{\text{input streams}} (c_{\text{HCl}} \dot{V}_{\text{HCl solution}})_{\text{in}} + r_{\text{formation,HCl}} = \sum_{\text{output streams}} (c_{\text{HCl}} \dot{V}_{\text{HCl solution}})_{\text{out}} + r_{\text{consumption,HCl}}
\]

\[
c_{\text{HCl}} = 0.014 \text{ M}
\]

\[
\dot{V}_{\text{HCl solution}} = 11600 \text{ L/hr}
\]

\[
\text{System}
\]

\[
c_{\text{HCl}} = c_{\text{NaOH}} = 0 \text{ M}
\]

\[
r_{\text{consumption,HCl}} = 1
\]

\[
r_{\text{consumption,NaOH}} = 1
\]

**Steady-State Mole Balance for NaOH**

\[
\sum_{\text{input streams}} (c_{\text{NaOH}} \dot{V}_{\text{NaOH solution}})_{\text{in}} + r_{\text{formation,NaOH}} = \sum_{\text{output streams}} (c_{\text{NaOH}} \dot{V}_{\text{NaOH solution}})_{\text{out}} + r_{\text{consumption,NaOH}}
\]

\[
\dot{V}_{\text{NaOH solution}} = \frac{c_{\text{HCl}} \dot{V}_{\text{HCl solution}}}{c_{\text{NaOH}}}
\]
Homework problem 1.

Feed water is fed to a large steady-state boiler. Most of the water leaves the boiler as high-pressure steam, with a smaller amount of hot residual water discharged to waste. The water densities and flow rates and the steam density are as follows:

<table>
<thead>
<tr>
<th>Stream</th>
<th>Density ((\text{kg/m}^3))</th>
<th>Volumetric Flow Rate ((\text{m}^3/\text{min}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed water</td>
<td>1000</td>
<td>28.0</td>
</tr>
<tr>
<td>Hot residual water</td>
<td>960</td>
<td>6.5</td>
</tr>
<tr>
<td>High-pressure steam</td>
<td>3.7</td>
<td></td>
</tr>
</tbody>
</table>

What is the volumetric flow rate of the steam?
Homework problem 5.

An “absorber” is a device used to bring a gas containing toxic chemicals into contact with a liquid that absorbs some of those toxic chemicals from the gas. Thus, a gas stream and liquid stream leave the absorber.

In an absorber you are designing, the entering gas stream flows at 340 \( \text{ft}^3/\text{min} \), while the gas stream leaving the absorber flows at 270 \( \text{ft}^3/\text{min} \). Meanwhile, the liquid stream leaving the absorber must be treated, so its flow rate is specified to be 77 \( \text{lb}_m/\text{min} \).

What mass flow rate is needed for the entering liquid stream (in units of \( \text{lb}_m/\text{min} \))?

The densities of the entering and exiting gas streams are equal to 0.087 \( \text{lb}_m/\text{ft}^3 \).
Homework problem 10.

Gas in a tank contains a poison at a concentration $c_T$, but the gas is leaking into the surrounding room at a rate of $T \text{ cm}^3/\text{min}$. Meanwhile, an air conditioner brings fresh air into the room at a rate of $A \text{ cm}^3/\text{min}$. The air in the room is well mixed and leaves through an open window (with the same concentration as in the room). The densities of all the gases are the same. Initially, the concentration of poison in the room ($c_R$) will rise, but it eventually will reach a steady value. In terms of the given symbols, what is that steady concentration?
Homework problem 13.

For the combustion of methane presented in Example 5.4, the chemical reaction is

$$\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$$

Suppose that methane flows into a burner at 30 $\text{gmol/s}$, while oxygen flows into the same burner at 75 $\text{gmol/s}$. If all the methane is burned and a single output stream leaves the burner, what is the mole fraction of $\text{CO}_2$ in that output stream?

Hint 1: Does the fact that all the methane is burned mean that all the oxygen is burned also?

Hint 2: Find the molar flow rate of each component gas in the outlet gas (“flue gas”).
Homework problem 16.

Fuel cells have been proposed for use in cars and for power generation as part of a hydrogen economy. They offer the advantages of higher efficiency (not limited by heat cycle efficiencies) and cleaner fuel with no significant pollutants. The net reaction is as follows:

\[ 2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} \]

where \( \text{O}_2 \) comes from the air (which, for this problem, can be assumed to be 21 mole\% \( \text{O}_2 \) and 79 mole\% \( \text{N}_2 \)). Hydrogen \( (\text{H}_2) \) flows into a fuel cell implemented in a prototype vehicle at a rate of 27 \( \text{gmol/min} \). Air (consisting of oxygen and nitrogen enters the fuel cell in a separate stream. The amount of oxygen entering the fuel cell is 50\% more than that needed to react stoichiometrically with all of the entering hydrogen. The conversion of hydrogen in the fuel cell is 85\%. Assume that only a single stream exits the fuel cell. What is the flow rate of each of the species leaving the fuel cell? Note that the flow rates given correspond to a fuel cell rated at approximately 50 \( \text{kW} \) using 2004 technology.
Homework problem 18.

Ammonia is used for fertilizer production and has been critical to successful agriculture. A steady-state chemical process is used to convert nitrogen (N\(_2\)) and hydrogen (H\(_2\)) to ammonia (NH\(_3\)) by the reaction

\[
N_2 + 3H_2 \rightarrow 2NH_3
\]

Stream 1, containing 95 mole\% nitrogen and 5 mole\% hydrogen, enters the process at a rate of 400 \(lbmol/hr\), and stream 2, containing pure hydrogen (density = 0.08 \(lb/ft^3\)), enters the process at a volumetric flow rate of 31000 \(ft^3/hr\). A single stream leaves the process. If all of the nitrogen is consumed in the reaction, what is the molar flow rate of hydrogen in the exiting stream?
Problem 05 (Mid-term Exam 2018)

(30 point) In order to produce high quality hydrogen from methane, two steady-state reactors are serially connected as shown in below.

For the Reactor 1, the methane steam reforming reaction occurs (CH\(_4\) + H\(_2\)O \rightarrow CO + 3H\(_2\)). The methane input flows into the Reactor 1 at a rate of 64.2 g/min. Water input enters the Reactor 1 in a separate stream. The amount of water entering the Reactor 1 is 25% more than that needed to react stoichiometrically with all of the entering methane. The conversion of methane in Reactor 1 is 75%.

For the Reactor 2, the water gas shift reaction occurs (CO + H\(_2\)O \rightarrow H\(_2\) + CO\(_2\)). The output from Reactor 1 flows into the Reactor 2. Another water input enters the Reactor 2 in a separate stream, in order to achieve the carbon monoxide conversion of 100%.

Assume that there is no side reaction in both of the Reactor 1 and 2.

(a) What is mole fraction of CO in the output from Reactor 1?
(b) What is the minimum molar flow rate of H\(_2\)O input 2 entering the Reactor 2? The answer should be given with unit of gmol/min.
(c) What is the mole fraction of H\(_2\) in the output from Reactor 2?